LEVEL II

INFORMAL
REPORT
NCSL 241-75

APRIL 1975

AD-A109 862

ON THE INVERSION OF THE MAGNETIC FIELD ℓ^{th} – DERIVATIVE EQUATIONS FOR A POINT 2^{ℓ} –POLE MAGNETIC FIELD

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ADMINISTRATIVE INFORMATION

This work was performed under the Independent Research Program ZR 000 01 01, Task 0401-36. The objective of the task is to study magnetic signal processing techniques.

Approved March 1974
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TABLE OF CONTENTS

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER NCSL ~~202-74~~ 241-75	2. GOVT ACCESSION NO. AD-A109867	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) ON THE INVERSION OF THE MAGNETIC FIELD ℓ^{th}-DERIVATIVE EQUATIONS FOR A POINT 2^{ℓ}-POLE MAGNETIC FIELD		5. TYPE OF REPORT & PERIOD COVERED Informal
		6. PERFORMING ORG. REPORT NUMBER April 1975
7. AUTHOR(s) Charles P. Frahm		8. CONTRACT OR GRANT NUMBER(s)
9. PERFORMING ORGANIZATION NAME AND ADDRESS Naval Coastal Systems Laboratory Panama City, Florida 32401		10. PROGRAM ELEMENT PROJECT TASK AREA & WORK UNIT NUMBERS ZR 000 01 01 Task 0401-36
11. CONTROLLING OFFICE NAME AND ADDRESS Naval Coastal Systems Laboratory Panama City, Florida 32401		12. REPORT DATE
		13. NUMBER OF PAGES 32
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office) Chief of Naval Material Navy Department Washington, D. C. 20360		15. SECURITY CLASS. (of this report) UNCLASSIFIED
		15a. DECLASSIFICATION DOWNGRADING SCHEDULE N/A

16. DISTRIBUTION STATEMENT (of this Report)

Approved for Public Release: Distribution Unlimited

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Differential Calculus
Magnetic Fields
Magnetic dipoles
Equations
Bearing (Direction)

Identifiers
Independent Research Program

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

(to the L power)

A general procedure is outlined for inverting the magnetic field derivative equations for a point 2^{ℓ}-pole magnetic field. The procedure is believed to be valid for arbitrary ℓ although an explicit proof has been obtained only for $\ell = 0$, 1, and 2. The details for $\ell = 2$ are included.

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S/N 0102-014-6601

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

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Utilization of the procedure permits a determination of the bearing of the source and the scaled multipole moments of the source; i.e., the moments divided by a power of the source-to-detector distance, from a knowledge of the field derivatives at a single space point only. The procedure makes use of a spherical basis representation in which only the independent multipole moments and field derivatives occur.

INTRODUCTION

It has been shown[1,2] that it is possible to invert the magnetic field first-derivative equations for a point-magnetic dipole field, thereby obtaining the bearing and scaled magnetic moments (quantities related to the magnetic moments) of the field source from a knowledge of the first field-derivatives at a single point only. This inversion of the first-derivative dipole equations can be done in closed form and is greatly facilitated by carrying out the analysis in the principle axis frame of the first field-derivative tensor. Unfortunately there seem to be no analogous special reference frames which simplify the analysis of the higher derivative equations for the corresponding higher multipole sources. However, by using a spherical tensor representation, wherein only the independent quadrupole moments and field derivatives appear, it is possible to formulate the inversion of the magnetic field second-derivative equations for a point quadrupole source in terms of two simultaneous transcendental equations which appear to be amenable to numerical solution on a digital computer. These equations have been solved numerically for several special cases. In each such special case it was found that there were not more than six solutions and that these solutions exhibited a certain degree of symmetry about the origin. If it is assumed that this is true, in general, for the quadrupole inversion problem it would indicate that there are three solutions in each half space, making a total of five ghost solutions and one physical solution. This is not substantially worse than the dipole inversion problem if the half-space in which the source resides is known a priori.

The spherical tensor procedure has also been shown to be applicable to a monopole source (for heuristic purposes only) and a dipole source. A recipe for inverting the dipole problem by the spherical tensor procedure is given in the appendix. The spherical tensor procedure is also

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(1) Naval Ship Research and Development Laboratory Report 3493, *Dipole Tracking with a Gradiometer,* by W. M. Wynn, January 1972, Unclassified.

(2) Naval Coastal Systems Laboratory Report 135-72, *Inversion of the Magnetic Field Gradient Equations for a Magnetic Dipole Field,* by C. P. Frahm, November 1972, Unclassified.

believed to be applicable to the magnetic field ℓth-derivative equations for a point 2^{ℓ}-pole source although a complete proof has not yet been established. In this report the general scheme of the procedure believed to be applicable to an arbitrary 2^{ℓ}-pole source will be presented followed by the details of the inversion for a quadrupole source.

MULTIPOLE FIELD DERIVATIVE EQUATIONS

In a static situation the magnetic field $\vec{H}$ produced by a magnetic source can be derived from a magnetic scalar potential ϕ by the familiar relation

$$\vec{H} = -\nabla\phi \tag{1}$$

Furthermore, if one is willing to introduce the fiction of magnetic poles, the potential can be conveniently expressed in the form

$$\phi(\vec{r}) = \int \frac{\rho(\vec{r}\,')}{|\vec{r} - \vec{r}\,'|} d^3r' \tag{2}$$

where $\rho(\vec{r}\,')$ is the magnetic pole density of the source at point $\vec{r}\,'$ and $\vec{r}$ is the observation point. (See Figure 1).

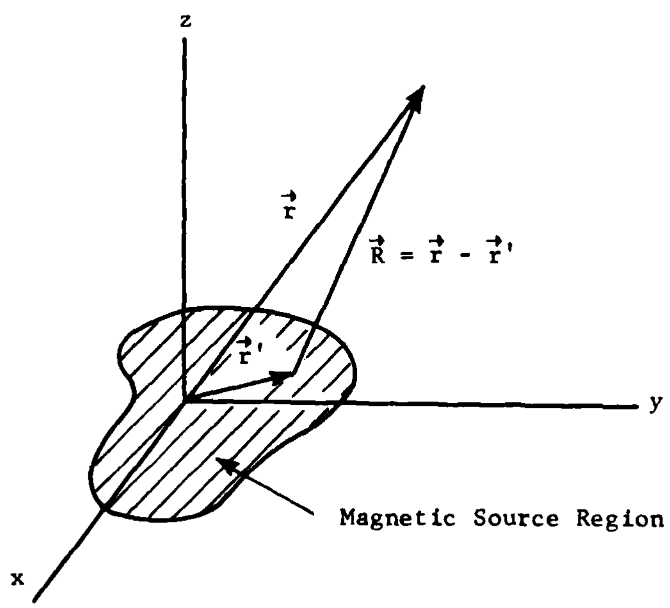

FIGURE 1. MAGNETIC FIELD SOURCE AND OBSERVATION POINTS

The multipole expansion of the scalar potential is then obtained by making a Taylor's series exapnsion of the factor

$$\frac{1}{|\vec{r} - \vec{r}'|} = \frac{1}{R} . \tag{3}$$

This gives

$$1/R = 1/r - x_i'\partial_i(1/r) + \frac{1}{2!} x_i'x_j'\partial_i\partial_j(1/r) + \ldots \tag{4a}$$

$$= \sum_{\ell=0}^{\infty} \frac{(-1)^\ell}{\ell!} x_{i_1}' x_{i_2}' \ldots x_{i_\ell}' \partial_{i_1} \partial_{i_2} \ldots \partial_{i_\ell} (1/r) . \tag{4b}$$

In Equation (4) the summation convention has been employed wherein repeated lower case subscripts are to be summed from 1 to 3 with the understanding that

$$x_1 = x,\ x_2 = v,\ x_3 = z \tag{5a}$$

and

$$\partial_1 = \partial/\partial x,\ \partial_2 = \partial/\partial y,\ \partial_3 = \partial/\partial z. \tag{5b}$$

The summation convention will be used throughout this report unless otherwise stated.

Using the expansion (4b) in the expression for the scalar potential Equation (2) gives

$$\phi(\vec{r}) = \sum_{\ell=0}^{\infty} \frac{(-1)^\ell}{\ell!} \partial_{i_1} \ldots \partial_{i_\ell} (1/r) \int \rho(\vec{r}') x_{i_1}' \ldots x_{i_\ell}' d^3r' . \tag{6}$$

The integrals

$$Q_{i_1 \ldots i_\ell} = \int \rho(\vec{r}') x_{i_1}' \ldots x_{i_\ell}' d^3r' \tag{7}$$

in Equation (6) are by construction completely symmetric *ℓth*-rank tensors and are occasionally referred to as multipole moments[3]. However,

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[3] Panofsky, W. K. H. and Phillips, M., *Classical Electricity and Magnetism,* p. 15, Addison-Wesley, 1955.

it is more convenient to define the 2^{ℓ}-pole moments in terms of the symmetric traceless part of $\tilde{Q}_{i_1 \ldots i_\ell}$. Such a symmetric traceless part can always be extracted from a tensor of rank 2 or higher and has the following form

$$Q_{i_1 \ldots i_\ell} = \frac{(2\ell)!}{2^{\ell}\ell!}\Bigg[\tilde{Q}_{i_1 \ldots i_\ell} + a\sum_{\alpha\beta} \delta_{i_\alpha i_\beta}\,\tilde{Q}\ldots \underbrace{i_\alpha \cdots i_\beta} \cdots$$

$$+ b\sum_{\alpha\beta}\sum_{\mu\lambda} \delta_{i_\alpha i_\beta}\,\delta_{i_\mu i_\lambda}\tilde{Q}\ldots \underbrace{i_\alpha \ldots i_\beta} \ldots \underbrace{i_\mu \ldots i_\lambda} \ldots$$

$$+ \ldots\Bigg] \tag{8}$$

where the coefficients a,b... are determined by the equations that result from setting the trace of $Q_{i_1 \ldots i_\ell}$ on any two indices equal to zero. The Greek indices take on the values $1,2 \ldots \ell$ and the following notation has been used to denote traces

$$A_{\underbrace{jk}} = A_{jj} \; . \tag{9}$$

The overall factor of $(2\ell)!/2^{\ell}\ell!$ has been introduced for later convenience.

For the special cases of $\ell = 1$, 2, and 3, Equation (8) gives the dipole moments

$$Q_i = \tilde{Q}_i = \int \rho(\vec{r})\; x_i d^3r \tag{10a}$$

the quadrupole moments

$$Q_{ij} = 3(\tilde{Q}_{ij} - \frac{1}{3}\,\delta_{ij}\,\tilde{Q}_{kk})$$

$$= \int \rho(\vec{r})\;(3x_i x_j - \delta_{ij} r^2)\; d^3r \tag{10b}$$

and the octupole moments

$$Q_{ijk} = 15[\tilde{Q}_{ijk} - \frac{1}{5}(\delta_{ij}\tilde{Q}_{mmk} + \delta_{ik}\tilde{Q}_{mjm} + \delta_{jk}\tilde{Q}_{imm})]$$

$$= \int \rho(\vec{r})\;[15x_i x_j x_k - 3(\delta_{ij}x_k + \delta_{ik}x_j + \delta_{jk}x_i)r^2]\; d^3r, \tag{10c}$$

respectively.

One interesting aspect of Equation (8) is that every term on the right side except the first involves at least one Kronecker delta which is to be contracted with the quantities $\partial_{i_1}\cdots\partial_{i_\ell}\,(1/r)$ in Equation (6). These terms will thus result in expressions involving derivatives of $\nabla^2(1/r)$ which is zero. Hence, it follows that

$$\phi(\vec{r}) = \sum_{\ell=0}^{\infty} \frac{(-1)^\ell}{\ell!}\,\partial_{i_1}\cdots\partial_{i_\ell}\,(1/r)\,\tilde{Q}_{i_1\ldots i_\ell}$$

$$= \sum_{\ell=0}^{\infty} \frac{(-1)^\ell 2^\ell}{(2\ell)!}\,\partial_{i_1}\cdots\partial_{i_\ell}(1/r)\,Q_{i_1\ldots i_\ell} \quad . \tag{11}$$

Now by a process of induction it can be shown that

$$\partial_{i_1}\cdots\partial_{i_\ell}(1/r) = \frac{(-1)^\ell\,(2\ell)!}{2^\ell\,\ell!}\,\frac{n_{i_1}\cdots n_{i_\ell}}{r^{\ell+1}} + \ldots \tag{12}$$

where the n_i are the direction cosines of $\vec{r}$; i.e.,

$$n_i = x_i/r \tag{13}$$

and the missing terms in Equation (12) all involve one or more Kronecker deltas on the indices $i_1 \ldots i_\ell$. Thus, when they are contracted with the traceless multipole moments in Equation (11) they give zero. Hence, Equation (11) reduces to

$$\phi(\vec{r}) = \sum_{\ell=0}^{\infty} \frac{1}{\ell!}\,Q_{i_1\ldots i_\ell}\,\frac{n_{i_1}\cdots n_{i_\ell}}{r^{\ell+1}} \quad . \tag{14}$$

For a pure 2^ℓ-pole source, only the ℓth term in the sum contributes and the potential has the form

$$\phi(\vec{r}) = \frac{1}{\ell!}\,Q_{i_1\ldots i_\ell}\,\frac{n_{i_1}\cdots n_{i_\ell}}{r^{\ell+1}} \quad . \tag{15}$$

The corresponding magnetic field components have the form

$$H_j = -\partial_j\phi = -\frac{1}{\ell!}\,Q_{i_1\ldots i_\ell}\,\partial_j\!\left(\frac{n_{i_1}\cdots n_{i_\ell}}{r^{\ell+1}}\right) \quad . \tag{16}$$

Taking ℓ derivatives of Equation (16) and introducing the notation

$$D_{j_1 \ldots j_{\ell+1}} = \partial_{j_1} \ldots \partial_{j_\ell} H_{j_{\ell+1}} \tag{17}$$

results in the field derivative equations for a 2^ℓ-pole source

$$D_{j_1 \ldots j_{\ell+1}} = q_{i_1 \ldots i_\ell} R_{i_1 \ldots i_\ell j_1 \ldots j_{\ell+1}} \tag{18}$$

where the $q_{i_1 \ldots i_\ell}$ are the scaled multipole moments defined by

$$q_{i_1 \ldots i_\ell} = Q_{i_1 \ldots i_\ell} / \ell ! r^{2(\ell+1)} \tag{19}$$

and $R_{i_1 \ldots i_\ell j_1 \ldots j_{\ell+1}}$ is a $(2\ell + 1)$-rank tensor defined by

$$R_{i_1 \ldots i_\ell j_1 \ldots j_{\ell+1}} = -r^{2(\ell+1)} \partial_{j_i} \ldots \partial_{j_{\ell+1}} (n_{i_1} \ldots n_{i_\ell} / r^{\ell+1}) \quad . \tag{20}$$

It will be convenient to introduce a notation that obviates the need for recording all of the subscripts. To accomplish this, parentheses will be used to denote a set of ℓ subscripted indices while square brackets will be used to denote a set of ℓ+1 subscripted indices. Thus,

$$R_{(i)[j]} = R_{i_1 \ldots i_\ell j_1 \ldots j_{\ell+1}} \quad . \tag{21}$$

Using this notation, the 2^ℓ-pole field ℓth-derivative equations take the form

$$D_{[j]} = q_{(i)} R_{(i)[j]} \quad . \tag{22}$$

GENERAL INVERSION PROCEDURE

In this section a procedure will be outlined which is believed to be of general applicability for the inversion of Equation (22). Although a complete proof of the validity of the procedure in general has not been established, the procedure is successful in inverting Equation (22) for the special cases of ℓ = 0, 1 and 2.

The objective is to use Equation (22) to determine the bearing $(-n_j)$ and the scaled moments $(q_{(i)})$ of a 2^{ℓ}-pole source from a knowledge of the field derivatives $(D_{[j]})$ at a single point. That this might be possible was first suggested by W. M. Wynn who noticed that the number of independent ℓth derivatives of the field components is $2\ell+3$, while the number of independent 2^{ℓ}-pole moments is $2\ell+1$, and the number of independent direction cosines (n_i) is 2 (except for a sign ambiguity). Thus, the number of independent pieces of information contained in the field derivatives is precisely the same as the number of independent unknowns. The number of independent components of $D_{[j]}$ and $q_{(i)}$ follow from the fact that they are both completely symmetric and traceless tensors.

The inversion procedure requires that two tensors $S_{(i)[j]}$ and $\tilde{N}_{[j](i)}$ be found with the following properties:

1. $q_{(i)} S_{(i)[j]} = 0$ (23)

2. $q_{(i)} N_{(i)[j]} \tilde{N}_{[j](k)} = q_{(k)}$ (24)

   where

$$N_{(i)[j]} = R_{(i)[j]} + S_{(i)[j]} \tag{25}$$

3. $\tilde{N}_{[j](i)} N_{(i)[k]}$ must be symmetric and traceless in the separate indices [j] and (k).

4. $\tilde{N}_{[j](i)} N_{(i)[k]}$ must be idempotent; i.e.,

$$\tilde{N}_{[j](i)} N_{(i)[\ell]} \tilde{N}_{[\ell](m)} N_{(m)[k]} = \tilde{N}_{[j](i)} N_{(i)[k]} \; . \tag{26}$$

By definition $R_{(i)[j]}$ is a dimensionless tensor which can only depend on the direction cosines n_i. Hence, $R_{(i)[j]}$ must be expressible as a sum of terms involving products of direction cosines and Kronecker deltas. From Equations (23-26) it then follows that $S_{(i)[j]}$ and $\tilde{N}_{[j](i)}$ must have similar forms. Thus, one can write the most general expressions with arbitrary coefficients and then adjust the coefficients to satisfy the above four conditions, thereby obtaining $S_{(i)[j]}$ and $\tilde{N}_{[j](i)}$.

Because of Equation (23), the field derivative equations can be written

$$D_{[j]} = q_{(i)} N_{(i)[j]} \; . \tag{27}$$

Then contracting on the right with $\tilde{N}_{[j](k)}$ yields by virtue of Equation (24)

$$q_{(k)} = D_{[j]} \tilde{N}_{[j](k)} \; . \tag{28}$$

Substituting this back into Equation (27) results in the equation

$$D_{[i]} = D_{[k]} \tilde{N}_{[k](\ell)} N_{(\ell)[i]} \; . \tag{29}$$

Equation (29) determines the direction cosines in terms of the field derivatives while Equation (28) gives the scaled moments in terms of the field derivatives and the direction cosines. Thus, the inversion is complete once Equation (29) is solved.

Relation (29) involves $2\ell+3$ equations for only two unknowns. Clearly many of these equations must be redundant if there is to be a solution. In order to explicitly see the independent equations in (29) it is convenient to change to a spherical tensor notation[4]. For any tensor of rank $\ell+1$ it is possible to construct linear combinations of the components which transform under rotations like objects of definite spin J and z-component M as follows

$$T^{(j)}_{JM} = K^{(j)JM}_{[i]} D_{[i]} \; . \tag{30}$$

The coefficients $K^{(j)JM}_{[i]}$ accomplish the transformation from the cartesian basis to the spherical basis and involve Clebsch-Gordan coefficients[4,5]. Since the construction of a spin J object with z-component M from a set of $\ell+1$ spin 1 objects (vectors) is usually not unique, the superscript set of $\ell-1$ indices (j) is needed to distinguish the various ways of making the composition[6].

In the special case where $D_{[i]}$ is completely symmetric and traceless (as it is in the current discussion), the construction is unique so that Equation (30) is identically zero unless

$$J = J_o = \ell+1 \tag{31a}$$

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[4] Rose, M. E., *Theory of Angular Momentum* (Wiley, 1957).

[5] Edmonds, A. R., *Angular Momentum in Quantum Mechanics* (Princeton University Press, 1957) Chapter 3.

[6] Racah, G., *in Ergebnisse der Exakten Naturwissenschaften,* Vol. 37, p. 56 (Springer-Verlag, 1965).

and

$$(j) = (j_o) \tag{31b}$$

where (j_o) is the unique set of indices that gives a non-zero result[a].

The spherical basis transformation coefficients form an orthonormal set

$$\bar{K}^{(j)JM}_{[i]} \; K^{(j')J'M'}_{[i]} = \delta_{(j)(j_o)} \; \delta_{JJ'} \; \delta_{MM'} \tag{32}$$

and a complete set

$$\sum_{(j)JM} K^{(j)JM}_{[k]} \; \bar{K}^{(j)JM}_{[\ell]} = \delta_{[k][\ell]} \tag{33}$$

where the bar denotes complex conjugation and

$$\delta_{(j)(j')} = \begin{cases} 1, \text{ if } (j) = (j') \\ o, \text{ otherwise} \end{cases} . \tag{34}$$

Equations (32) and (33) follow from the completeness and orthonormality properties of the Clebsch-Gordan coefficients themselves.

Now by contracting with $K^{(j)JM}_{[i]}$ and inserting Equation (33) on the right side Equation (29) becomes

$$D_{[i]}K^{(j)JM}_{[i]} = \sum_{(j')J'M'} D^{(j')J'M'}_{[k]} \; \bar{K}^{(j')J'M'}_{[\ell]} \; \tilde{N}_{[\ell](m)} \; N_{(m)[i]} \; K^{(j)JM}_{[i]} . \tag{35}$$

As pointed out in Equation (31) this is a non-trivial result only when $(j) = (j_o)$ and $J=J_o$. Furthermore, the sum on the right side contributes only when $(j') = (j_o)$ and $J' = J_o$. Thus the non-trivial part of Equation (35) can be written

$$T_M = T_{M'} \; V_{M'M} \tag{36}$$

---

[a] In the usual parlance of quantum theory, the only way to obtain a total spin of $\ell+1$ by combining $\ell+1$ spin 1 objects is to make all the spins parallel.

or in matrix notation

$$T = TV \qquad (37)$$

where

$$T_M = D_{[i]} K_{[i]}^{(j_o)J_oM} \qquad (38)$$

and

$$V_{M'M} = \bar{K}_{[\ell]}^{(j_o)J_oM'} \tilde{N}_{[\ell](m)} N_{(m)[i]} K_{[i]}^{(j_o)J_oM} . \qquad (39)$$

In Equation (36) and subsequent equations, the summation convention is extended to repeated upper case subscripts. These will be understood to be summed from 1 to $2J_o+1$.

The $(2J_o+1)$ X $(2J_o+1)$ matrix $V_{M'M}$ is idempotent as can be seen from Equations (39), (33), and (26) and from the comments accompanying Equation (31). Thus

$$V_{M'M''} V_{M''M} = V_{M'M} \qquad (40)$$

In the special cases $\ell = 0$, 1, and 2 the V-matrix is also hermitian

$$\bar{V}_{M'M} = V_{MM'} \qquad (41)$$

and has a trace given by

$$V_{MM} = 2J_o - 1 = 2\ell+1 . \qquad (42)$$

Thus, it is possible in these cases to diagonalize the V-matrix by a similarity transformation with a unitary matrix and obtain diagonal elements consisting of $2\ell+1$ ones and 2 zeroes. Furthermore, it was found in these special cases that it was always possible to perform an appropriate coordinate rotation described by Euler angles (α,β,γ) and thereby diagonalize the associated V-matrix. Assuming these results to be valid for arbitrary ℓ, implies that the unitary matrix that diagonalizes the V-matrix is the rotation matrix $D_{MM'}^{(J)}$ (α,β,γ) belonging to the *Jth* irreducible representation of the rotation group (Chapter 4 of Reference 5)[b].

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[b] It should also be noted that for the rotation matrices the superscript symbol (J) denotes only one index and not a set of indices. This and the two usages of D (compare Equation (17) and (45)) should cause no confusion.

Performing the similarity transformation on V in Equation (37) results in the equation

$$t = tV_d \tag{43}$$

where V_d is the diagonal form of V

$$(V_d)_{M'M} = [D^{(J)}_{M'M''}(\alpha,\beta,\gamma)]^{-1} V_{M''M'''} [D^{(J)}_{M'''M}(\alpha,\beta,\gamma)] \tag{44}$$

and

$$t_M = T_{M'} D^{(J)}_{M'M}(\alpha,\beta,\gamma) \ . \tag{45}$$

For the unit diagonal elements in V_d Equation (43) reduces to an identity. However, the two zero diagonal elements give two non-trivial complex equations of the form

$$t_{M_1} = 0 \tag{46a}$$

$$t_{M_2} = 0 , \tag{46b}$$

where M_1 and M_2 are defined by

$$(V_d)_{M_1M_1} = (V_d)_{M_2M_2} = 0 \text{ (no sum)} \ . \tag{47}$$

The two equations in Equation (46) are not independent as can be seen from the fact that the usual choice of phases for the Clebsch-Gordan coefficients gives

$$\overline{K}^{(j_o)J_oM}_{[i]} = (-1)^M K^{(j_o)J_o-M}_{[i]} \tag{48}$$

so that

$$\overline{T}_M = (-1)^M T_{-M} \ . \tag{49}$$

Furthermore,

$$\overline{D}^{(J)}_{M'M}(\alpha,\beta,\gamma) = (-1)^{M'-M} D^{(J)}_{-M'-M}(\alpha,\beta,\gamma) \tag{50}$$

so that

$$\bar{t}_M = (-1)^M t_{-M} . \tag{51}$$

Thus, if

$$t_{M_1} = 0 \tag{52a}$$

it follows that

$$t_{-M_1} = 0 . \tag{52b}$$

But there are only two zeroes on the diagonal of V_d so that it must be concluded that

$$M_1 = -M_2 \tag{53}$$

and only one of the equations in (46) is independent.

Now the two real equations resulting from the complex equation[c]

$$t_{M_1} = 0 \tag{54}$$

are the two independent equations referred to earlier which can be solved (at least numerically) for the Euler angles once the field derivatives are known. After the Euler angles are known, the direction cosines can be written immediately (refer to discussion leading to Equation (111)).

$$n_1 = -\sin\beta \cos\gamma \tag{55a}$$

$$n_2 = \sin\beta \sin\gamma \tag{55b}$$

$$n_3 = \cos\beta \tag{55c}$$

---

[c] The choice of M_1 in Equation (54) seems to be arbitrary. However, at least for ℓ=2, it is most expedient to choose $M_1 = J_o$ (see Equation (89) ff.).

QUADRUPOLE INVERSION

For a point quadrupole source (ℓ=2) the potential is given by Equation (15)

$$\phi(\vec{r}) = \frac{1}{2} Q_{ij} n_i n_j / r^3 \quad . \tag{56}$$

Taking the negative gradient gives the magnetic field

$$H_k = \frac{1}{2} Q_{ij} (5 n_i n_j n_k - \delta_{ik} n_j - \delta_{jk} n_i)/r^4 \quad . \tag{57}$$

Two additional derivatives then yield

$$D_{m\ell k} = q_{ij} R_{ijk\ell m} \tag{58}$$

with

$$D_{m\ell k} = \partial_m \partial_\ell H_k \tag{59a}$$

$$q_{ij} = Q_{ij}/2r^6 \tag{59b}$$

$$\begin{aligned} R_{ijk\ell m} = {} & 5[63 R^1_{ijk\ell m} - 7(R^2_{ijk\ell m} + R^3_{ijk\ell m}) \\ & + R^4_{ijk\ell m} + R^5_{ijk\ell m}] \end{aligned} \tag{59c}$$

and

$$R^1_{ijk\ell m} = n_i n_j n_k n_\ell n_m \tag{60a}$$

$$R^2_{ijk\ell m} = n_i n_j (\delta_{km} n_\ell + \delta_{\ell m} n_k + \delta_{k\ell} n_m) \tag{60b}$$

$$\begin{aligned} R^3_{ijk\ell m} = {} & n_k n_\ell (\delta_{im} n_j + \delta_{jm} n_i) + n_k n_m (\delta_{i\ell} n_j + \delta_{j\ell} n_i) \\ & + n_\ell n_m (\delta_{ik} n_j + \delta_{jk} n_i) \end{aligned} \tag{60c}$$

$$\begin{aligned} R^4_{ijk\ell m} = {} & n_i (\delta_{\ell j} \delta_{km} + \delta_{k\ell} \delta_{jm} + \delta_{jk} \delta_{\ell m}) \\ & + n_j (\delta_{\ell i} \delta_{km} + \delta_{k\ell} \delta_{im} + \delta_{ik} \delta_{\ell m}) \end{aligned} \tag{60d}$$

$$R^5_{ijk\ell m} = n_k(\delta_{i\ell}\delta_{jm} + \delta_{j\ell}\delta_{im}) + n_\ell(\delta_{ik}\delta_{jm} + \delta_{jk}\delta_{im})$$

$$+ n_m(\delta_{ik}\delta_{j\ell} + \delta_{jk}\delta_{i\ell}) \ . \qquad (60e)$$

In constructing the tensors $S_{(i)[j]}$ and $\tilde{N}_{[j](i)}$ it is also necessary to consider terms of the form

$$R^6_{ijk\ell m} = \delta_{ij} n_k n_\ell n_m \qquad (60f)$$

$$R^7_{ijk\ell m} = (n_i\delta_{jk} - n_j\delta_{ik})\, n_\ell n_m + (n_i\delta_{j\ell} - n_j\delta_{i\ell})\, n_k n_m$$

$$+ (n_i\delta_{jm} - n_j\delta_{im})\, n_k n_\ell \qquad (60g)$$

$$R^8_{ijk\ell m} = \delta_{ij}(n_k\delta_{\ell m} + n_\ell\delta_{km} + n_m\delta_{k\ell}) \qquad (60h)$$

$$R^9_{ijk\ell m} = (n_i\delta_{jk} - n_j\delta_{ik})\, \delta_{\ell m} + (n_i\delta_{j\ell} - n_j\delta_{i\ell})\, \delta_{km}$$

$$+ (n_i\delta_{jm} - n_j\delta_{im})\, \delta_{k\ell} \ . \qquad (60i)$$

All of the quantities $R^n_{ijk\ell m}$ are symmetric in $(k\ell m)$ and either symmetric or antisymmetric in (ij). These are the only such quantities that can be constructed as sums of products of Kronecker deltas and direction cosines. Furthermore, these are the only types of quantities that can occur in $S_{(i)[j]}$ and $\tilde{N}_{[j](i)}$ because of condition 3. Thus, it is reasonable to attempt to construct $S_{(i)[j]}$ and $N_{[j](i)}$ in the forms

$$S_{ijk\ell m} = \sum_{n=1}^{9} a_n R^n_{ijk\ell m} \qquad (61a)$$

and

$$\tilde{N}_{k\ell mij} = \sum_{n=1}^{9} b_n R^n_{ijk\ell m} \ . \qquad (61b)$$

After a lot of algebra one can determine the coefficients a_n and b_n from the four conditions discussed in the previous section. The results are

$$a_6 = -10 \qquad (62a)$$

$$a_n = 0, \text{ for } n \neq 6 \tag{62b}$$

and

$$b_1 = 1/8 \tag{63a}$$

$$b_2 = -1/1500 \tag{63b}$$

$$b_3 = -1/24 \tag{63c}$$

$$b_4 = 1/600 \tag{63d}$$

$$b_5 = 1/60 \tag{63e}$$

$$b_6 = 1/24 \tag{63f}$$

$$b_n = 0, \text{ for } n = 7, 8, 9. \tag{63g}$$

Contracting $\tilde{N}_{k\ell mst}$ with

$$N_{ijk\ell m} = R_{ijk\ell m} + S_{ijk\ell m} \tag{64}$$

gives

$$N_{ijk\ell m}\,\tilde{N}_{k\ell mst} = \frac{1}{2}(\delta_{is}\delta_{jt} + \delta_{js}\delta_{it}) + \frac{1}{4}\,\delta_{ij}n_s n_t - \frac{5}{12}\,\delta_{ij}\delta_{st} \tag{65}$$

and

$$\tilde{N}_{rstij}\,N_{ijk\ell m} = \sum_{n=1}^{9} C_n\,T^n_{rstk\ell m} \tag{66}$$

where

$$T^1_{rstk\ell m} = n_r n_s n_t n_k n_\ell n_m \tag{67a}$$

$$T^2_{rstk\ell m} = n_r n_s n_t(\delta_{km}n_\ell + \delta_{\ell m}n_k + \delta_{k\ell}n_m) \tag{67b}$$

$$\begin{aligned} T^3_{rstk\ell m} = {} & n_r n_s(n_k n_\ell \delta_{tm} + n_k n_m \delta_{t\ell} + n_m n_\ell \delta_{tk}) \\ & + n_r n_t(n_k n_\ell \delta_{sm} + n_k n_m \delta_{s\ell} + n_m n_\ell \delta_{sk}) \\ & + n_t n_s(n_k n_\ell \delta_{rm} + n_k n_m \delta_{r\ell} + n_m n_\ell \delta_{rk}) \end{aligned} \tag{67c}$$

$$
\begin{aligned}
T^4_{rstk\ell m} = {} & n_r n_s(\delta_{k\ell}\delta_{tm} + \delta_{km}\delta_{t\ell} + \delta_{m\ell}\delta_{tk}) \\
& + n_r n_t(\delta_{k\ell}\delta_{sm} + \delta_{km}\delta_{s\ell} + \delta_{m\ell}\delta_{sk}) \\
& + n_t n_s(\delta_{k\ell}\delta_{rm} + \delta_{km}\delta_{r\ell} + \delta_{m\ell}\delta_{rk}) \qquad (67d)
\end{aligned}
$$

$$
\begin{aligned}
T^5_{rstk\ell m} = {} & n_r[n_k(\delta_{s\ell}\delta_{tm} + \delta_{sm}\delta_{t\ell}) + n_\ell(\delta_{sk}\delta_{tm} + \delta_{tk}\delta_{sm}) \\
& + n_m(\delta_{sk}\delta_{t\ell} + \delta_{tk}\delta_{s\ell})] + n_s[n_k(\delta_{r\ell}\delta_{tm} + \delta_{rm}\delta_{t\ell}) \\
& + n_\ell(\delta_{rk}\delta_{tm} + \delta_{tk}\delta_{rm}) + n_m(\delta_{rk}\delta_{t\ell} + \delta_{tk}\delta_{r\ell})] \\
& + n_t[n_k(\delta_{s\ell}\delta_{rm} + \delta_{sm}\delta_{r\ell}) + n_\ell(\delta_{sk}\delta_{rm} + \delta_{rk}\delta_{sm}) \\
& + n_m(\delta_{sk}\delta_{r\ell} + \delta_{rk}\delta_{s\ell})] \qquad (67e)
\end{aligned}
$$

$$T^6_{rstk\ell m} = (n_r\delta_{st} + n_s\delta_{rt} + n_t\delta_{rs})\, n_k n_\ell n_m \qquad (67f)$$

$$T^7_{rstk\ell m} = (n_r\delta_{st} + n_s\delta_{rt} + n_t\delta_{rs})(n_\ell\delta_{km} + n_k\delta_{\ell m} + n_m\delta_{k\ell}) \qquad (67g)$$

$$
\begin{aligned}
T^8_{rstk\ell m} = {} & n_k n_\ell(\delta_{rs}\delta_{tm} + \delta_{rt}\delta_{sm} + \delta_{st}\delta_{rm}) \\
& + n_\ell n_m(\delta_{rs}\delta_{tk} + \delta_{rt}\delta_{sk} + \delta_{st}\delta_{rk}) \\
& + n_k n_m(\delta_{rs}\delta_{t\ell} + \delta_{rt}\delta_{s\ell} + \delta_{st}\delta_{r\ell}) \qquad (67h)
\end{aligned}
$$

$$
\begin{aligned}
T^9_{rstk\ell m} = {} & (\delta_{r\ell}\delta_{km} + \delta_{k\ell}\delta_{rm} + \delta_{rk}\delta_{\ell m})\, \delta_{st} \\
& + (\delta_{s\ell}\delta_{km} + \delta_{k\ell}\delta_{sm} + \delta_{ks}\delta_{\ell m})\, \delta_{rt} \\
& + (\delta_{tk}\delta_{\ell m} + \delta_{\ell t}\delta_{km} + \delta_{k\ell}\delta_{tm})\, \delta_{rs} \qquad (67i)
\end{aligned}
$$

and

$$C_1 = C_2 = -C_3 = C_6 = \frac{1}{4} \qquad (68a)$$

$$C_4 = C_7 = C_8 = -\frac{1}{12} \qquad (68b)$$

$$C_5 = \frac{1}{6} \tag{68c}$$

$$C_9 = \frac{1}{60} \tag{68d}$$

Using Equations (61a), (62a), and (65-68) it is fairly easy to determine that the four conditions of the previous section are indeed satisfied by Equations (61-63). As shown in the previous section, these conditions are sufficient to establish Equations (28) and (29) which for the quadrupole case become

$$q_{ij} = D_{k\ell m} \tilde{N}_{k\ell mij} \tag{69}$$

and

$$D_{k\ell m} = D_{rst} \tilde{N}_{rstij} N_{ijk\ell m}, \tag{70}$$

respectively.

The spherical basis transformation coefficients for $\ell = 2$ are given by

$$K^{jJM}_{ik\ell} = \sum_{m_i} (1m_1jm_4|1jJM)(1m_21m_3|11jm_4)U_{m_1i}U_{m_2k}U_{m_3\ell} \tag{71}$$

where $(j_1m_1j_2m_2|j_1j_2jm)$ is the Clebsch-Gordan coefficient[d] for coupling spin j_1 and spin j_2 to obtain spin j with z-component m; and U is the unitary matrix which converts the cartesian vector components to spherical vector components (page 66 of Reference 4).

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & -i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & -i & 0 \end{pmatrix} . \tag{72}$$

---

[d] Edmonds notations (Reference 5) will be used for the Clebsch-Gordan coefficients throughout this report.

The rows of U are labeled from top to bottom by the spherical index $m = 1, 0, -1$ while the columns are labeled from left to right by the cartesian index $i = 1, 2, 3$.

Since U is unitary its inverse is given by

$$U^{-1} = U^{\dagger} = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & 0 & 1 \\ i & 0 & i \\ 0 & \sqrt{2} & 0 \end{pmatrix} \tag{73}$$

where the rows are now labeled by the cartesian index and the columns by the spherical index. Furthermore, by inspection of Equation (72) it is easily seen that

$$U_{-mi} = (-1)^m \bar{U}_{mi} \ . \tag{74}$$

The Clebsch-Gordan coefficients satisfy an orthogonality relation

$$\sum_{m_1 m_2} (j_1 m_1 j_2 m_2 | j_1 j_2 JM)(j_1 m_1 j_2 m_2 | j_1 j_2 J'M') = \delta_{JJ'} \delta_{MM'} \tag{75a}$$

and a completeness relation

$$\sum_{JM} (j_1 m_1 j_2 m_2 | j_1 j_2 JM)(j_1 m_1' j_2 m_2' | j_1 j_2 JM) = \delta_{m_1 m_1'} \delta_{m_2 m_2'} \tag{75b}$$

as well as a number of symmetry properties including[5]

$$(j_1 -m_1 j_2 -m_2 | j_1 j_2 J -M) = (-1)^{j_1 + j_2 - J} (j_1 m_1 j_2 m_2 | j_1 j_2 JM) \tag{75c}$$

$$(j_2 m_2 j_1 m_1 | j_2 j_1 JM) = (-1)^{j_1 + j_2 - J} (j_1 m_1 j_2 m_2 | j_1 j_2 JM) \ . \tag{75d}$$

---

[5] Edmonds, A. R., *Angular Momentum in Quantum Mechanics*, Princeton University Press 1957, Chapter 3.

Using these relations along with Equations (72) and (73), it is straightforward to establish a number of useful relations for the spherical basis transformation coefficients.

$$\bar{K}^{jJM}_{ik\ell}\, K^{j'J'M'}_{ik\ell} = \delta_{jj'}\delta_{JJ'}\delta_{MM'} \tag{76a}$$

$$\sum_{jJM} K^{jJM}_{ik\ell}\, \bar{K}^{jJM}_{rst} = \delta_{ir}\delta_{ks}\delta_{\ell t} \tag{76b}$$

$$K^{jJ-M}_{ik\ell} = (-1)^{J+M+1}\, \bar{K}^{jJM}_{ik\ell} \; . \tag{76c}$$

In addition it can be established that for the special case j=2, J=3 the spherical basis transformation coefficients are completely symmetric[e] and traceless; i.e.,

$$K^{23M}_{ik\ell} = K^{23M}_{i\ell k} = K^{23M}_{ki\ell} \tag{77a}$$

and

$$K^{23M}_{ikk} = 0 \quad . \tag{77b}$$

As discussed in the previous section the relations (76b) are sufficient to permit rewriting equation (70) in the form

$$T_M = T_{M'}V_{M'M} \tag{78}$$

where

$$T_M = D_{k\ell m}K^{23M}_{k\ell m} \, , \tag{79}$$

and

$$V_{M'M} = \bar{K}^{23M'}_{rst}\; \tilde{N}_{rstij}\; N_{ijk\ell m}\; K^{23M}_{k\ell m} \; . \tag{80}$$

---

[e] The establishment of the last equality in Equations (77a) is not quite so straightforward since it requires a recombination of the three spins involved; these can best be handled by using Racah's W-coefficients or Wigner's 6-j symbols. See E. P. Wigner, *Group Theory* (Academic Press, 1959), Equation 24.24.

It is not necessary to explicitly evaluate the right side of Equation (80) in terms of the direction cosines although this could be done. Instead it is only necessary to establish a few properties of the V-matrix from the defining relation (80); namely, that V has a trace of 5, is hermitian, and is idempotent[f].

The hermiticity of V is established as follows

$$V_{M'M} = \bar{K}^{23M'}_{[r]} \tilde{N}_{[r](i)} N_{(i)[s]} K^{23M}_{[s]}$$

$$= \sum_{n=1}^{9} C_n \bar{K}^{23M'}_{[r]} T^{n}_{[r][s]} K^{23M}_{[s]} \text{, from Equation (66)}$$

$$= \sum_{n=1,3,5} C_n \bar{K}^{23M'}_{[r]} T^{n}_{[r][s]} K^{23M}_{[s]} \text{, from Equations (67) and (77).}$$

Now by inspection of Equations (67) it is seen that

$$T^{n}_{[r][s]} = T^{n}_{[s][r]} \text{, for } n = 1,\ 3,\ 5 \text{ .} \tag{81}$$

Thus,

$$V_{M'M} = \sum_{n=1,3,5} C_n K^{23M}_{[s]} T^{n}_{[s][r]} \bar{K}^{23M'}_{[r]} = V_{MM'} \text{ .} \tag{82}$$

The idempotent property is established by using the idempotent character of $\tilde{N}_{[r](i)} N_{(i)[s]}$ along with Equation (76b) and the comment associated with Equations (31).

---

[f] V has another curious property that follows from Equation (76c).

$$V_{-M-M'} = (-1)^{M+M'} \bar{V}_{MM'}$$

However, this relation is of no utility in the present discussion.

$$V_{M'M''} V_{M''M} = \sum_{M''} \bar{K}^{23M'}_{[r]} \tilde{N}_{[r](i)} N_{(i)[s]} K^{23M''}_{[s]}$$

$$\times \bar{K}^{23M''}_{[t]} \tilde{N}_{[t](j)} N_{(j)[u]} K^{23M}_{[u]}$$

$$= \sum_{jJM''} \bar{K}^{23M'}_{[r]} \tilde{N}_{[r](i)} N_{(i)[s]} K^{jJM''}_{[s]}$$

$$\times \bar{K}^{jJM''}_{[t]} \tilde{N}_{[t](j)} N_{(j)[u]} K^{23M}_{[u]}$$

$$= \bar{K}^{23M'}_{[r]} \tilde{N}_{[r](i)} N_{(i)[s]} \tilde{N}_{[s](j)} N_{(j)[u]} K^{23M}_{[u]}$$

$$= \bar{K}^{23M'}_{[r]} \tilde{N}_{[r](i)} N_{(i)[u]} K^{23M}_{[u]}$$

$$= V_{M'M} \ . \tag{83}$$

The trace of V is evaluated in a similar fashion

$$V_{MM} = \sum_{M} \bar{K}^{23M}_{[r]} \tilde{N}_{[r](i)} N_{(i)[s]} K^{23M}_{[s]}$$

$$= \sum_{jJM} \bar{K}^{jJM}_{[r]} \tilde{N}_{[r](i)} N_{(i)[s]} K^{23M}_{[s]}$$

$$= \delta_{[r][s]} \tilde{N}_{[r](i)} N_{(i)[s]} = \tilde{N}_{[r](i)} N_{(i)[r]}$$

$$= \sum_{n=1}^{9} C_n T^n_{[r][r]} \ . \tag{84}$$

The quantities $T^n_{[r][r]}$ can be evaluated from Equations (67) with the result

$$V_{MM} = 5 \ . \tag{85}$$

The hermiticity of V implies that V can be diagonalized by a similarity transformation with a unitary matrix. The resulting diagonal matrix V_d by virtue of the idempotent property of V can have only ones and zeroes on the diagonal. Finally, the trace relation (85) requires that there be exactly five ones and two zeroes on the diagonal of V_d.

The position of the zeroes on the diagonal can be established by considering a special case. When the vector $\vec{r}$ lies along the z-axis; i.e.,

$$n_\ell = \delta_{\ell 3} \; . \tag{86}$$

The explicit form of the V-matrix can be determined using Equations (67) and (68) in the relation

$$V_{M'M} = \sum_{n=1,3,5} C_n \, \bar{K}^{23M'}_{rst} \, T^n_{rstk\ell m} \, K^{23M}_{k\ell m} \tag{87}$$

which was obtained in arriving at Equation (82). For this special case one finds that

$$V = V_d = (0,\ 1,\ 1,\ 1,\ 1,\ 1,\ 0) \tag{88}$$

where the last equality gives the elements along the diagonal. From this result one learns not only the order of the elements in V_d, but also that the unitary matrix that diagonalizes the V-matrix corresponds to a rotation of coordinates that brings the z-axis into coincidence with $\vec{r}$. This implies that the diagonalizing matrix belongs to a representation of the rotation group and hence is one of the rotation matrices $D^{(3)}_{MM'}(\alpha,\beta,\gamma)$ where (α,β,γ) are the Euler angles of the desired rotation. Thus,

$$[D^{(3)}(\alpha,\beta,\gamma)]^{-1}\, V D^{(3)}(\alpha,\beta,\gamma) = V_d = (0,1,1,1,1,1,0) \tag{89}$$

for some choice of (α,β,γ).

(NB: When diagonalizing an hermitian matrix by a unitary matrix, the order of the resulting diagonal elements is usually immaterial. However, if the positions of the zeroes in Equations (88) and (89) are altered, it is no longer clear that the diagonalizing matrix is one of the matrices $D^{(3)}(\alpha,\beta,\gamma)$. Thus, to ensure that the diagonalizing matrix is one of these matrices and not some other unitary 7X7 matrix, it is expedient to adopt the order given.)

To determine the appropriate values of the Euler angles the rotation is applied to Equation (78) yielding

$$t = tV_d \tag{90}$$

where

$$t = TD^{(3)}(\alpha,\beta,\gamma) \; . \tag{91}$$

For the components $M = 0$, ± 1, and ± 2, Equation (90) is a trivial identity. However, for $M = \pm 3$ it imposes the following conditions on (α, β, γ)

$$t_{\pm 3} = 0 \ . \tag{92}$$

As pointed out in the previous section, only one of these complex equations is independent since Equations (79) and (76c) imply that

$$T_{-M} = (-1)^M \, \overline{T}_M \ . \tag{93}$$

Thus, it is sufficient to consider only

$$t_3 = 0 \ . \tag{94}$$

Using the notation of Edmonds (Chapter 4 of Reference 5) for the rotation matrix, Equation (94) becomes

$$\sum_M T_M \, e^{iM\gamma} \, d^{(3)}_{M3}(\beta) e^{i3\alpha} = 0 \ . \tag{95}$$

Clearly the value of α is arbitrary so that Equation (95) imposes two real conditions on the two angles β and γ.

$$\sum_M T_M e^{iM\gamma} \, d^{(3)}_{M3}(\beta) = 0 \ . \tag{96}$$

The two real conditions imposed by Equation (96) can be explicitly exhibited in a convenient way by using Equation (93) and writing

$$T_M = \rho_M e^{i\theta_M} \tag{97}$$

with ρ_M and θ_M both real. Thus, (suppressing the argument β)

$$\begin{aligned}
&\sum_M T_M e^{iM\gamma} d^{(3)}_{M3} \\
&\quad = T_o d^{(3)}_{o3} + \sum_{M=1}^{3} \left[T_M e^{iM\gamma} d^{(3)}_{M3} + T_{-M} e^{-iM\gamma} d^{(3)}_{-M3} \right] \\
&\quad = \rho_o d^{(3)}_{o3} + \sum_{M=1}^{3} \rho_M \left[e^{i(\theta_M + M\gamma)} \ d^{(3)}_{M3} + (-1)^M \ e^{-i(\theta_M + M\gamma)} d^{(3)}_{-M3} \right] \\
&\quad = 0 \ .
\end{aligned} \tag{98}$$

Taking the real and imaginary parts of this last equality gives the desired conditions.

$$\rho_0 d_{03}^{(3)} + \sum_{M=1}^{3} \rho_M \cos(\theta_M + M\gamma)[d_{M3}^{(3)} + (-1)^M d_{-M3}^{(3)}] = 0 \qquad (99a)$$

$$\sum_{M=1}^{3} \rho_M \sin(\theta_M + M\gamma)[d_{M3}^{(3)} - (-1)^M d_{-M3}^{(3)}] = 0 \ . \qquad (99b)$$

The $d_{M3}^{(3)}(\beta)$ are given in Chapter 4 of Reference 5.

$$d_{M3}^{(3)}(\beta) = -(-1)^M \left[\frac{6!}{(3-M)!(3+M)!}\right]^{\frac{1}{2}} \cos^{3+M} \beta/2 \sin^{3-M} \beta/2 \ . \qquad (100)$$

Thus,

$$d_{33}^{(3)}(\beta) = \cos^6 \beta/2 \qquad (101a)$$

$$d_{23}^{(3)}(\beta) = -\sqrt{6} \cos^5 \beta/2 \sin \beta/2 \qquad (101b)$$

$$d_{13}^{(3)}(\beta) = \sqrt{15} \cos^4 \beta/2 \sin^2 \beta/2 \qquad (101c)$$

$$d_{03}^{(3)}(\beta) = -2\sqrt{5} \cos^3 \beta/2 \sin^3 \beta/2 \qquad (101d)$$

$$d_{-13}^{(3)}(\beta) = \sqrt{15} \cos^2 \beta/2 \sin^4 \beta/2 \qquad (101e)$$

$$d_{-23}^{(3)}(\beta) = -\sqrt{6} \cos \beta/2 \sin^5 \beta/2 \qquad (101f)$$

$$d_{-33}^{(3)}(\beta) = \sin^6 \beta/2 \ . \qquad (101g)$$

Defining

$$A_M = d_{M3}^{(3)}(\beta) + (-1)^M d_{-M3}^{(3)}(\beta) \qquad (102a)$$

and

$$B_M = d_{M3}^{(3)}(\beta) - (-1)^M d_{-M3}^{(3)}(\beta), \qquad (102b)$$

one finds

$$1/2\ A_0 = d^{(3)}_{03} = -\frac{\sqrt{5}}{4} \sin^3 \beta \tag{103a}$$

$$A_1 = \frac{\sqrt{15}}{4} \sin^3 \beta \cot \beta \tag{103b}$$

$$A_2 = \frac{\sqrt{6}}{4} \sin^3 \beta (1 + 2 \cot^2 \beta) \tag{103c}$$

$$A_3 = \frac{1}{4} \sin^3 \beta \cot \beta (3 + 4 \cot^2 \beta) \tag{103d}$$

$$B_1 = \frac{\sqrt{15}}{4} \sin^2 \beta \tag{103e}$$

$$B_2 = \frac{6}{2} \sin^2 \beta \cot \beta \tag{103f}$$

$$B_3 = \frac{1}{4} \sin^2 \beta (1 + 4 \cot^2 \beta) . \tag{103g}$$

Using Equations (102-103) and defining

$$\chi = \cot \beta, \tag{104}$$

Equations (99), after some simplification, become

$$\begin{aligned} \sin^3 \beta [&\rho_3 \chi (3 + 4\chi^2) \cos(\theta_3 + 3\gamma) \\ &- \sqrt{6}\, \rho_2 (1 + 2\chi^2) \cos(\theta_2 + 2\gamma) \\ &+ \sqrt{15}\, \rho_1 \chi \cos(\theta_1 + \gamma) - \sqrt{5}\, \rho_0] = 0 \end{aligned} \tag{105a}$$

$$\begin{aligned} \sin^2 \beta\ [&\rho_3 (1 + 4\chi^2) \sin(\theta_3 + 3\gamma) \\ &- 2\sqrt{6}\, \rho_2 \chi \sin(\theta_2 + 2\gamma) \\ &+ \sqrt{15}\ \rho_1 \sin(\theta_1 + \gamma)] = 0 . \end{aligned} \tag{105b}$$

Solution of these two equations for β(or χ) and γ then permits the completion of the inversion process. Unfortunately these equations are transcendental and do not seem to permit a simple solution. They are

probably best solved numerically once the values of ρ_M and θ_M are known. Only solutions in the ranges

$$0 \leq \beta \leq \pi \tag{106a}$$

$$0 \leq \gamma < 2\pi \tag{106b}$$

need be determined. Once the solutions of Equations (105) are known the direction cosines n_j can be easily determined.

The spherical basis components Y_m of n_j are given according to Equations (30) and (71) by

$$Y_m = U_{mi} n_i \ . \tag{107}$$

In the special frame where $n_i = \delta_{i3}$ (denoted by a prime) this gives

$$Y'_m = U_{m3} = \delta_{mo} \ . \tag{108}$$

By Equation (91) Y'_m and Y_m are related by

$$Y'_m = Y_{m'} D^{(3)}_{m'm} (\alpha,\beta,\gamma) \ . \tag{109}$$

Solving Equations (107-109) for n_i gives

$$n_i = U^{-1}_{im} [D^{(1)}_{om} (\alpha,\beta,\gamma)]^{-1} \ . \tag{110}$$

Explicit evaluation of Equation (110) using Edmond's expression for $D^{(1)}(\alpha,\beta,\gamma)$ gives

$$n_1 = -\sin \beta \cos \gamma \tag{111a}$$

$$n_2 = \sin \beta \sin \gamma \tag{111b}$$

$$n_3 = \cos \beta \ . \tag{111c}$$

It is now straightforward to evaluate the scaled moments q_{ij} from Equation (69), thus completing the inversion process for the quadrupole source.

NB: It should be noted that the terms involving $R^2_{ijk\ell m}$ and $R^4_{ijk\ell m}$ do not contribute to the sum in Equation (69) because of the traceless character of $D_{k\ell m}$. Furthermore, the evaluation of the remaining sums can be greatly simplified by taking advantage of the symmetry of $D_{k\ell m}$.

SUMMARY OF THE QUADRUPOLE INVERSION RECIPE

Once the values of the independent second derivatives (for example D_{111}, D_{112}, D_{113}, D_{122}, D_{123}, D_{222}, D_{223}) are known, the spherical components can be computed from Equation (79). After considerable simplification these give

$$T_3 = -\sqrt{2}/2[D_{111} - 3D_{122} + i(3D_{112} - D_{222})] \quad (112a)$$

$$T_2 = \sqrt{3}/2[D_{113} - D_{223} + 2i\, D_{123}] \quad (112b)$$

$$T_1 = \sqrt{30}/4[D_{111} + D_{122} + i(D_{112} + D_{222})] \quad (112c)$$

$$T_o = -\sqrt{10}/2[D_{113} + D_{223}] \ . \quad (112d)$$

The moduli ρ_M and arguments θ_M can then be computed from the real and imaginary parts of T_M in the usual way.

$$\rho_M = [(\mathrm{Re}\ T_M)^2 + (\mathrm{Im}\ T_M)^2]^{\frac{1}{2}} \quad (113a)$$

$$\sin\theta_M = \mathrm{Im}\ T_M/\rho_M,\ \cos\theta_M = \mathrm{Re}\ T_M/\rho_M\ . \quad (113b)$$

These can then be substituted into Equations (105) and the resulting equations solved for β and γ in the intervals specified in relations (106).

For convenience, the pertinent equations are repeated here.

$$\sin^3\beta[\rho_3\chi(3 + 4\chi^2)\cos(\theta_3 + 3\gamma)$$

$$-\sqrt{6}\,\rho_2(1 + 2\chi^2)\cos(\theta_2 + 2\gamma)$$

$$+\sqrt{15}\,\rho_1\chi\cos(\theta_1 + \gamma) - \sqrt{5}\,\rho_o] \quad (105a)$$

$$\sin^2\beta[\rho_3(1 + 4\chi^2)\sin(\theta_3 + 3\gamma)$$

$$-2\sqrt{6}\,\rho_2\chi\sin(\theta_2 + 2\gamma)$$

$$+\sqrt{15}\,\rho_1\sin(\theta_1 + \gamma)] \quad (105b)$$

$$0 \leq \beta \leq \pi \tag{106a}$$

$$0 \leq \gamma < 2\pi \ . \tag{106b}$$

Finally, the direction cosines are given by Equations (111)

$$n_1 = -\sin \beta \cos \gamma \tag{111a}$$

$$n_2 = \sin \beta \sin \gamma \tag{111b}$$

$$n_3 = \cos \beta \tag{111c}$$

and the scaled quadrupole moments are given by Equations (69), (61b), (60) and (63). After much simplification the latter give[g]

$$q_{ij} = \frac{1}{10} n_m D_{mij} - \frac{1}{8}(n_j n_k n_\ell D_{k\ell i} + n_i n_k n_\ell D_{k\ell j})$$
$$+ \frac{1}{8}(n_i n_j + \frac{1}{3} \delta_{ij}) n_k n_\ell n_m D_{k\ell m} \quad . \tag{114}$$

For purposes of checking the results, the field derivatives can be regenerated using Equations (58) through (60). When combined these can be simplified to give

$$D_{k\ell m} = 5\{7[9n_k n_\ell n_m - (\delta_{km} n_\ell + \delta_{\ell m} n_k + \delta_{k\ell} n_m)] n_i n_j q_{ij}$$
$$+ 2[(-7n_k n_\ell + \delta_{k\ell}) n_j q_{jm} + (-7n_k n_m + \delta_{km}) n_j q_{j\ell}$$
$$+ (-7n_\ell n_m + \delta_{\ell m}) n_j q_{jk}]$$
$$+ 2(n_k q_{\ell m} + n_\ell q_{km} + n_m q_{k\ell})\} \ . \tag{115}$$

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[g] See comments following Equation (111).

APPENDIX A

DIPOLE INVERSION RECIPE
USING THE SPHERICAL TENSOR PROCEDURE

From the independent field derivatives (D_{11}, D_{12}, D_{13}, D_{22}, D_{23}), evaluate the spherical components T_M.

$$T_2 = \frac{1}{2}(D_{11} - D_{22} + 2iD_{12}) \tag{A1a}$$

$$T_1 = -(D_{13} + iD_{23}) \tag{A1b}$$

$$T_o = -\sqrt{2/3}\ (D_{11} + D_{22})\ . \tag{A1c}$$

The moduli ρ_M and arguments θ_M can then be evaluated in the usual way

$$\rho_M = [(\mathrm{Re}\ T_M)^2 + (\mathrm{Im}\ T_M)^2]^{\frac{1}{2}} \tag{A2a}$$

$$\sin\theta_M = \mathrm{Im}\ T_M/\rho_M,\ \cos\theta_M = \mathrm{Re}\ T_M/\rho_M\ . \tag{A2b}$$

The angles β and γ are then obtained by solving the following system of equations

$$\sin^2\beta[2\rho_2(1 + 2\chi^2)\cos(\theta_2 + 2\gamma)$$
$$-4\rho_1\chi\cos(\theta_1 + \gamma) + \sqrt{6}\ \rho_o] = 0 \tag{A3a}$$

$$\sin\beta[\rho_2\chi\ \sin(\theta_2 + 2\gamma) - \rho_1\ \sin(\theta_1 + \gamma)] = 0 \tag{A3b}$$

with

$$0 \leq \beta \leq \pi \tag{A4a}$$

$$0 \leq \gamma < 2\pi\ . \tag{A4b}$$

The direction cosines are given by

$$n_1 = -\sin\beta\ \cos\gamma \tag{A5a}$$

$$n_2 = \sin\beta\ \sin\gamma \tag{A5b}$$

$$n_3 = \cos\beta\ . \tag{A5c}$$

The scaled dipole moments are given by

$$q_{\ell} = \frac{1}{3} n_k D_{k\ell} - \frac{1}{2} n_{\ell} n_j n_k D_{jk} \ . \tag{A6}$$

For checking purposes the field derivatives are regenerated by

$$D_{jk} = 3[(-5n_j n_k + \delta_{jk}) \ n_i q_i + n_j q_k + n_k q_j] \ . \tag{A7}$$

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